A Numerical Model for Etching through a Circular hole

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Abstract. A numerical model based on the total concentration of etchant is proposed to model the wet chemical etching through a circular hole. The reaction at the etchant-substrate interface is assumed to be infinitely fast i.e. etching is controlled by the diffusion of etchant to the interface. The proposed model is based on a fixed-grid approach analogous to the enthalpy method. The total concentration of etchant is the sum of the unreacted etchant concentration and the reacted etchant concentration. The reacted concentration of etchant is a measure of the etchfront position during etching. The governing mass diffusion equation based on the total concentration of etchant includes the interface condition. The etchfront position is found implicitly using the proposed approach. The computational domain is fixed, which includes the whole etchant and substrate domain including the mask region. For demonstration purposes, the finite volume method is used to solve the governing mass diffusion equation with prescribed initial and boundary conditions. The effect of mask thickness and initial etchant concentration on the shape evolution of etchfront is studied.

Keywords: wet chemical etching; total concentration; fixed-grid approach.

1. Introduction

Wet chemical etching (WCE) is a widely used material removal technique in microfabrication of different micro-devices[1],[2]. When etching progresses, the etched interface (etchant-substrate interface) moves and takes a definite shape in multidimensional etching depending on the etching condition. The shape of the etched interface gradually changes with time. Therefore, predicting and understanding the shape evolution of etchfront is important in designing a specific pattern on the substrate surface for its use in fabricating different micro-devices.

Existing approaches to model the WCE process includes the analytical asymptotic solution developed by Kuiken[3],[4], the moving grid (MG) numerical approach first developed by Vuik and Cuvelier[5] and subsequently by other researchers[6], the level-set method developed by Adalsteinsson and Sethian[7] and the recently introduced total concentration fixed-grid approach developed by Chai and his co-workers[8]-[10]. Although there is significant development found in the modeling of complex etching process since last two decades but very few existing models are there to model the wet etching process in circular geometries[4],[6].

Recently, Chai and his co-workers[8]-[10] developed a fixed-grid method based on the total concentration of etchant. This method is analogous to the enthalpy method[11],[12], widely used in the modeling of melting/solidification problems. The total concentration is the sum of the unreacted etchant concentration and the reacted etchant concentration. The conventional WCE problem is reformulated based on the total concentration of etchant. The modified governing equation includes the interface condition. The etchfront position can be found implicitly using this method. The reacted concentration of etchant is a measure of the etchfront position during etching. Since the grid size is fixed, there is no grid velocity unlike MG method. Simple Cartesian grid can be used to capture the complicated etch profile evolved during multidimensional WCE. The model has been successfully applied to one-dimensional[8],[9] and two-dimensional[10] WCE problems in rectangular geometries.

In this article, the total concentration based fixed-grid (FG) method is extended to model the WCE process in circular geometries. The effect of initial etchant concentration and mask thickness on the evolution of etch profile is investigated.

2. The Axisymmetric WCE Problem

The schematic of etching through a circular hole is shown in Fig. 1a. A circular cavity of diameter $2R$ is to be etched in a substrate covered with inert mask at the top. It can be treated as an axisymmetric problem as etching is uniform along angular direction at any radial location. The etching is assumed diffusion limited where reaction at the interface is infinitely fast. The origin of the co-ordinate system is set to the etchant-substrate interface at the center of the cavity. Since the problem is symmetric about the axis of symmetry, only half of the domain is considered as shown in Fig. 1b. The governing equation, the initial condition, the boundary conditions, and the interface condition are given below.

$$\frac{\partial c}{\partial t} = \frac{1}{r}\frac{\partial}{\partial r}\left(rD\frac{\partial c}{\partial r}\right) + \frac{\partial}{\partial z}\left(D\frac{\partial c}{\partial z}\right) \quad \text{in } \Omega\,(t),\ t > 0 \qquad \text{(1a)}$$

The initial and boundary conditions are

$$c = c_o \text{ in } \Omega\,(0),\ t = 0 \qquad \text{(1b)}$$

$$\frac{\partial c}{\partial r} = 0 \qquad \text{at } \Gamma_1,\ t > 0 \qquad \text{(1c)}$$

$$\frac{\partial c}{\partial \hat{n}} = 0 \qquad \text{at } \Gamma_4,\ t > 0 \qquad \text{(1d)}$$

$$c = c_o \text{ at } \Gamma_2 \text{ and } \Gamma_3,\ t > 0 \qquad \text{(1e)}$$

$$c = 0 \text{ on } f(t),\ t > 0 \qquad \text{(1f)}$$

The interface condition governing the normal speed of unknown moving interface $f(t)$ is given as

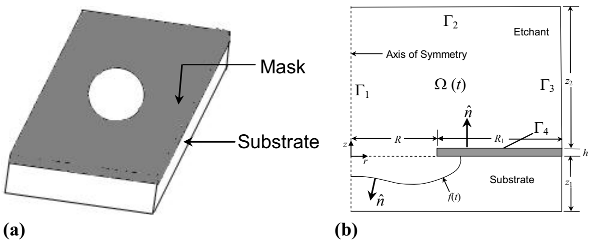

Fig. 1. The schematic and the computational domain: (a) the schematic of a circular hole to be etched in a substrate covered with inert mask; (b) the computational domain.

$$\mathrm{v}_{\hat{n}} = -\frac{DM_{Sub}}{m\rho_{Sub}}\frac{\partial c}{\partial \hat{n}} \qquad \text{on } f(t),\ t > 0 \qquad (2)$$

where D is the diffusion coefficient of etchant, M_{Sub} is the molecular weight of substrate, ρ_{Sub} is the density of substrate and m is the stoichiometric reaction parameter.

3. The Total Concentration Formulation

The total concentration of etchant c_{T} is defined as

$$c_{\mathrm{T}} \equiv c + c_{\mathrm{R}} \qquad (3)$$

where c is the unreacted etchant concentration and c_{R} is the reacted concentration of etchant. The value of c_{R} changes from 0 to its maximum possible value $c_{\mathrm{R,max}}$ in a control volume where etching is taking place called as ECV. The ECVs are the substrate control volumes with adjacent etchant control volumes. The $c_{\mathrm{R,max}}$ is expressed as

$$c_{\mathrm{R,max}} = \frac{m\rho_{Sub}}{M_{Sub}} \qquad (4)$$

The governing equation based on the total concentration is given as

$$\frac{\partial c_{\mathrm{T}}}{\partial t} = \frac{1}{r}\frac{\partial}{\partial r}\left(rD\frac{\partial c}{\partial r}\right) + \frac{\partial}{\partial z}\left(D\frac{\partial c}{\partial z}\right) \qquad (5)$$

Equation (5) is the modified governing equation which includes the interface condition (Eq. 2). How the interface condition can be extracted from the modified governing equation is derived in the previous articles on this method[9],[10]. Combining Eq. (3) and Eq. (5), gives

$$\frac{\partial c}{\partial t} = \frac{1}{r}\frac{\partial}{\partial r}\left(rD\frac{\partial c}{\partial r}\right) + \frac{\partial}{\partial z}\left(D\frac{\partial c}{\partial z}\right) - \frac{\partial c_{\mathrm{R}}}{\partial t} \qquad (6)$$

3.1. Procedure to Update c_R

c_{R} changes from 0 to its maximum possible value $c_{\mathrm{R,max}}$ in an etching-control-volume (ECV) where etching is taking place. An ECV is said to be etched completely when c_{R} reaches $c_{\mathrm{R,max}}$. Using the similar update procedure as discussed in previous articles on this method for diffusion-limited etching[8],[10], c_{R} can be updated iteratively as

$$c_{\mathrm{R},P}^{m+1} = c_{\mathrm{R},P}^{m} + \alpha\, a_P \frac{\Delta t}{\Delta V_P} c_P^m \qquad (7)$$

where α is the underrelaxation factor ($0 \le \alpha \le 1$), a is coefficient of the discretized equation, Δt is the time step size, ΔV is the volume of a control volume, subscript P is the control volume P and the superscript m is the m^{th} iteration of current time step. The only difference in the present axisymmetric etching problem is the volume of the control volume which is given as

$$\Delta V = r\Delta r\Delta z \qquad (8)$$

4. Numerical Method

The finite volume method (FVM) of Patankar[13] is used to solve the modified governing equation (Eq. 6). The detailed discussion on FVM can be found in Patankar[13]. The overall solution procedure is same as discussed in the previous articles[8]-[10].

5. Results and Discussions

The schematic of the axisymmetric etching model is shown in Fig. 1a. The governing equation is non-dimensionalized using following variables.

$$r^* = \frac{r}{R},\ Z = \frac{z}{R},\ t^* = \frac{tD}{R^2},\ C = \frac{c}{c_o},\ C_R = \frac{c_R}{c_o},\ \beta = \frac{m\rho_{Sub}}{c_o M_{Sub}} \quad (9)$$

where β is the dimensionless etching parameter. The dimensionless radial thickness of the mask is taken as $R_1^* = R_1 / R = 6.5$. The dimensionless height of the substrate to be etched and the etchant domain are taken as $Z_1 = z_1 / R = 0.5$ and $Z_2 = z_2 / R = 6.5$ respectively. Results for two mask thicknesses, namely,- infinitely thin and finite mask thickness are discussed. For infinitely thin mask, the dimensionless mask thickness is taken as $H = h / R = 0.005$. Further decrease in mask thickness does not alter the solution. For finite mask thickness, the thickness of the mask is taken as $H = h / R = 0.5$.

A grid refinement study was performed to ensure the solutions to be grid independent- both temporal as well as spatial. Figure 2a shows the evolution of etch profiles for three control volume sizes ranging from coarser to refined grids. For each control volume size, the time independent etch profiles are shown. The time step size is found to be $\Delta t^* = 0.01$. It is seen from Fig. 2a that, the grid sizes of 60 × 56 and 110 × 101 produced the same etch profiles. The bulging effect is seen near the mask corner where the etch rate is higher compared to the etch rate at the center of the cavity. This is because of the high concentration gradient near the mask corner due to high rate of diffusion of etchant. This is evident from the concentration contour plot shown in Fig. 2b where the contours goes deep near the mask corner in the etched region.

Figure 3a shows the evolution of etch profiles for finite mask thickness. It is seen that, the etch profiles are nearly uniform whole along the opened cavity region and there is no bulging effect seen near the corner of the mask. This is because of the uniform normal concentration gradient along the interface, due to larger diffusion length of the etchant from the area above the inert mask to the etching surface. As a result, the concentration contours are also uniform as shown in Fig. 3b. The underetching below the mask also reduced when mask thickness increases which can be seen by comparing Figs. 2a and 3a.

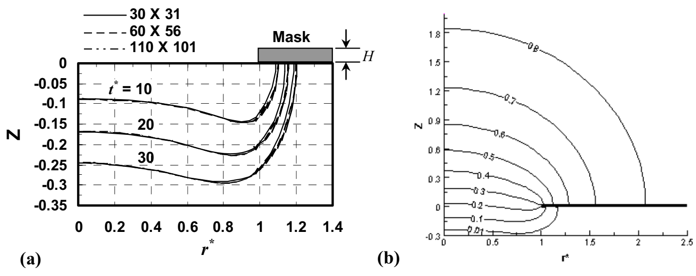

Fig. 2. The etchfront evolution and concentration distribution for β = 100 and infinitely thin mask (H = 0.005): (a) grid-independent study; (b) concentration contours at t^* = 30.

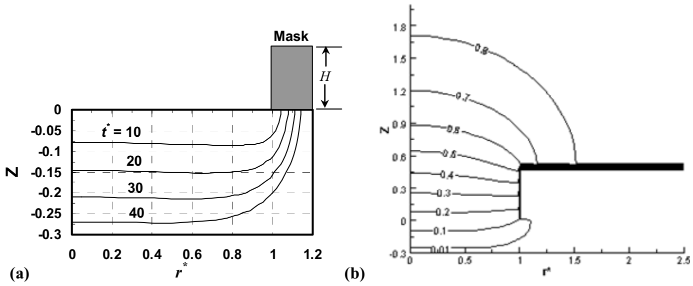

Fig. 3. Etchfront evolution and concentration distribution for $\beta = 100$ and finite mask thickness (H = 0.5): (a) etch profiles at four different times; (b) concentration contours at $t^* = 40$.

Figure 4 shows the shape evolution of etchfronts at t^* = 30 for three different initial etchant concentrations. As discussed before, the etching parameter β is a measure of the initial etchant concentration. For a given substrate to be etched β is inversely proportional to the initial etchant concentration c_o. Three β values are chosen to study the effect of initial etchant concentration on etchfront evolution. As expected, it is seen that the etch rate is higher and the etch profile goes deep as the initial etchant concentration increases. Also the bulging near the mask corner is less pronounced as initial etchant concentration increases.

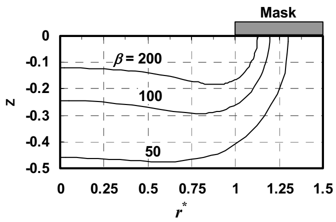

Fig. 4. Effect of β on etchfront evolution at t^* = 30.

6. Concluding Remarks

A total concentration fixed-grid method is applied to model the axisymmetric etching problem. With this method there is no necessity to capture the etchfront explicitly unlike the existing MG method. The method is applied for etching under diffusion limited condition. The effect of mask thickness and initial etchant concentration on etchfront evolution is studied. The underetching can be minimized by increasing the thickness of the mask and the etch rate can be increased by increasing the initial etchant concentration.

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